Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:08 PM EST

PDB ID	:	9D7Q
Title	:	Water and chloride as allosteric inhibitors in WNK kinase osmosensing
Authors	:	Akella, R.; Goldsmith, E.J.
Deposited on	:	2024-08-16
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

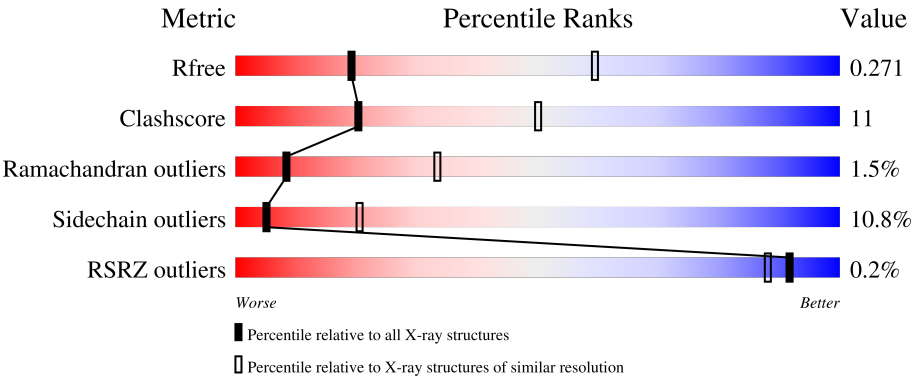
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	66% 24% • • 5%
1	B	280	72% 19% • • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4372 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase WNK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2143	1371	362	393	17			
1	B	265	Total	C	N	O	S	0	0	1
			2120	1358	363	383	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASN	ASP	conflict	UNP Q9BYP7
A	314	ALA	GLU	engineered mutation	UNP Q9BYP7
A	325	PHE	TYR	conflict	UNP Q9BYP7
B	279	ASN	ASP	conflict	UNP Q9BYP7
B	314	ALA	GLU	engineered mutation	UNP Q9BYP7
B	325	PHE	TYR	conflict	UNP Q9BYP7

- Molecule 2 is water.

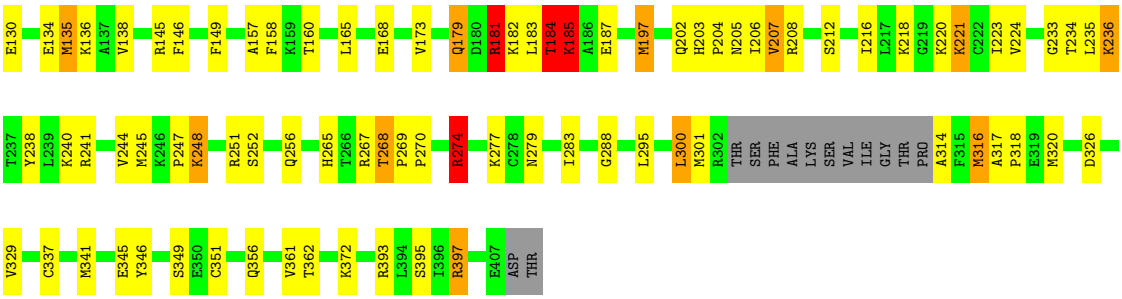
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total	O	0	0
			57	57		
2	B	52	Total	O	0	0
			52	52		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

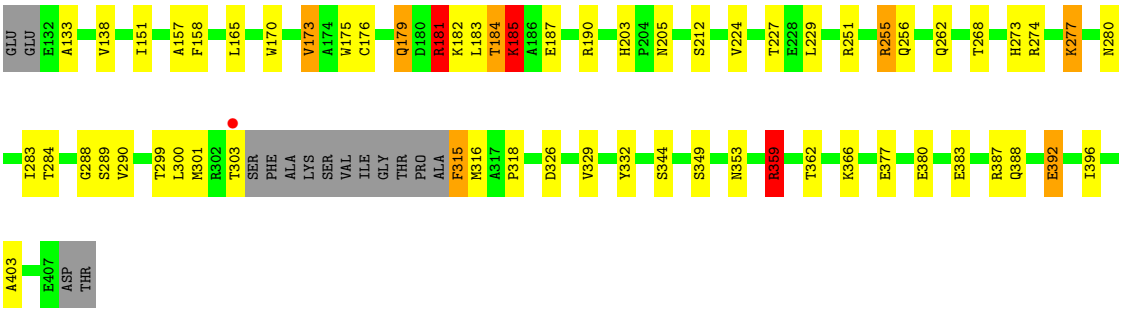
• Molecule 1: Serine/threonine-protein kinase WNK3

Chain A:



• Molecule 1: Serine/threonine-protein kinase WNK3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.17Å 113.60Å 67.52Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	43.11 – 3.30 43.11 – 3.30	Depositor EDS
% Data completeness (in resolution range)	70.0 (43.11-3.30) 70.1 (43.11-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.177 , 0.270 0.177 , 0.271	Depositor DCC
R_{free} test set	531 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	81.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4372	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/2186	0.89	3/2940 (0.1%)
1	B	0.35	0/2163	0.91	2/2909 (0.1%)
All	All	0.35	0/4349	0.90	5/5849 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	397	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	B	359	ARG	CD-NE-CZ	5.55	131.38	123.60
1	A	274	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	280	ASN	CB-CA-C	5.37	121.13	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	274	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	397	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	181	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2160	55	0
1	B	2120	0	2144	47	0
2	A	57	0	0	6	0
2	B	52	0	0	10	0
All	All	4372	0	4304	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:CYS:HB3	2:A:501:HOH:O	1.70	0.92
1:A:134:GLU:HB3	2:A:522:HOH:O	1.69	0.91
1:A:158:PHE:HB3	1:A:179:GLN:HB2	1.57	0.86
1:A:356:GLN:HB2	2:A:501:HOH:O	1.76	0.86
1:B:185:LYS:HB3	2:B:505:HOH:O	1.82	0.80
1:A:317:ALA:HB3	1:B:329:VAL:HG23	1.67	0.74
1:A:361:VAL:HG13	1:B:318:PRO:HG3	1.68	0.73
1:A:179:GLN:HB3	1:A:181:ARG:HH21	1.53	0.73
1:A:205:ASN:O	1:A:206:ILE:HD13	1.90	0.71
1:A:326:ASP:O	1:A:329:VAL:HG12	1.93	0.67
1:B:403:ALA:HB3	2:B:506:HOH:O	1.96	0.66
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.61	0.66
1:B:315:PHE:O	1:B:315:PHE:CD1	2.49	0.65
1:A:267:ARG:NE	1:A:267:ARG:HA	2.15	0.59
1:B:303:THR:CA	2:B:527:HOH:O	2.50	0.59
1:A:346:TYR:O	1:A:349:SER:OG	2.21	0.59
1:A:314:ALA:CB	1:B:277:LYS:NZ	2.66	0.58
1:B:326:ASP:O	1:B:329:VAL:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:HH21	1:B:359:ARG:HG2	1.71	0.55
1:B:284:THR:OG1	1:B:288:GLY:HA3	2.07	0.55
1:A:265:HIS:O	1:A:270:PRO:HB3	2.07	0.55
1:A:223:ILE:HD13	1:A:300:LEU:HD21	1.88	0.55
1:B:366:LYS:HE2	1:B:383:GLU:HG2	1.88	0.54
1:B:359:ARG:HH21	1:B:359:ARG:CG	2.19	0.54
1:B:273:HIS:O	1:B:274:ARG:HB2	2.07	0.54
1:A:207:VAL:O	1:A:295:LEU:HD11	2.08	0.54
1:A:314:ALA:HB2	1:B:277:LYS:NZ	2.23	0.53
1:A:316:MET:CE	2:B:527:HOH:O	2.56	0.53
1:B:185:LYS:HD2	2:B:533:HOH:O	2.08	0.53
1:B:255:ARG:NH1	1:B:255:ARG:CG	2.71	0.53
1:B:133:ALA:HB1	1:B:170:TRP:CH2	2.43	0.53
1:A:235:LEU:O	1:A:238:TYR:HB3	2.09	0.52
1:A:135:MET:HG2	1:A:136:LYS:N	2.24	0.52
1:A:223:ILE:HG21	1:A:300:LEU:HD13	1.92	0.52
1:B:158:PHE:O	1:B:179:GLN:HB2	2.10	0.52
1:A:317:ALA:HA	1:B:332:TYR:CD2	2.46	0.51
1:A:288:GLY:HA2	2:A:530:HOH:O	2.10	0.51
1:A:247:PRO:HD2	1:A:248:LYS:HE2	1.92	0.51
1:A:149:PHE:HZ	1:A:165:LEU:HD12	1.77	0.50
1:B:184:THR:O	1:B:185:LYS:HB2	2.11	0.50
1:B:255:ARG:HH11	1:B:255:ARG:CG	2.24	0.50
1:A:248:LYS:HD3	1:A:248:LYS:H	1.77	0.50
1:A:223:ILE:HG21	1:A:300:LEU:CD1	2.43	0.49
1:A:236:LYS:HD2	1:A:279:ASN:HB3	1.93	0.49
1:A:314:ALA:HB1	1:B:277:LYS:NZ	2.26	0.49
1:B:256:GLN:OE1	1:B:289:SER:HB2	2.12	0.49
1:B:362:THR:O	1:B:388:GLN:NE2	2.45	0.49
1:A:149:PHE:CZ	1:A:165:LEU:HD12	2.49	0.48
1:A:244:VAL:HG12	1:A:245:MET:N	2.29	0.48
1:A:203:HIS:CG	1:A:204:PRO:HD2	2.48	0.48
1:A:318:PRO:C	1:A:320:MET:H	2.17	0.47
1:A:184:THR:O	1:A:185:LYS:HB2	2.15	0.47
1:A:197:MET:HA	1:A:197:MET:CE	2.45	0.47
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.51	0.46
1:B:251:ARG:O	1:B:255:ARG:HB2	2.14	0.46
1:A:316:MET:HE3	2:B:527:HOH:O	2.12	0.46
1:A:212:SER:HA	1:A:224:VAL:O	2.15	0.46
1:B:377:GLU:O	1:B:380:GLU:HG2	2.16	0.46
1:B:212:SER:HA	1:B:224:VAL:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:CB	2:B:505:HOH:O	2.51	0.46
1:B:349:SER:HB3	2:B:520:HOH:O	2.16	0.46
1:A:337:CYS:O	1:A:341:MET:HG3	2.16	0.45
1:A:146:PHE:HA	1:A:165:LEU:O	2.15	0.45
1:B:173:VAL:HG22	1:B:227:THR:O	2.16	0.45
1:B:344:SER:HB3	2:B:501:HOH:O	2.17	0.45
1:A:317:ALA:CB	1:B:329:VAL:HG23	2.43	0.45
1:B:181:ARG:HD2	1:B:181:ARG:HA	1.46	0.45
1:B:315:PHE:CD1	1:B:315:PHE:C	2.89	0.45
1:B:190:ARG:HH11	1:B:299:THR:HG23	1.82	0.45
1:B:283:ILE:HG22	1:B:290:VAL:HG12	1.99	0.44
1:B:185:LYS:HA	1:B:185:LYS:HD3	1.56	0.44
1:A:145:ARG:HG3	1:A:168:GLU:HG3	1.99	0.44
1:A:345:GLU:OE2	1:A:372:LYS:HD2	2.18	0.44
1:A:216:ILE:HD13	1:A:221:LYS:HA	2.00	0.44
1:A:274:ARG:HH21	1:A:274:ARG:HG3	1.83	0.43
1:A:268:THR:HA	1:A:269:PRO:HA	1.79	0.43
1:B:387:ARG:HD3	1:B:392:GLU:HB3	2.00	0.43
1:A:248:LYS:H	1:A:248:LYS:CD	2.30	0.43
1:B:315:PHE:O	1:B:315:PHE:HD1	2.02	0.43
1:A:318:PRO:O	1:A:320:MET:N	2.51	0.43
1:B:173:VAL:HA	1:B:229:LEU:HB2	2.00	0.42
1:B:283:ILE:HA	1:B:289:SER:O	2.18	0.42
1:A:233:GLY:HA2	2:A:536:HOH:O	2.20	0.42
1:A:220:LYS:HD3	1:A:220:LYS:HA	1.67	0.42
1:B:262:GLN:HB2	1:B:396:ILE:HG21	2.02	0.42
1:A:267:ARG:NE	1:A:267:ARG:CA	2.83	0.42
1:B:203:HIS:HE1	1:B:205:ASN:HD22	1.67	0.41
1:A:251:ARG:HD2	2:A:514:HOH:O	2.19	0.41
1:A:252:SER:O	1:A:256:GLN:HG3	2.20	0.41
1:B:359:ARG:HH21	1:B:359:ARG:CB	2.33	0.41
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.83	0.41
1:B:185:LYS:C	2:B:505:HOH:O	2.59	0.41
1:A:318:PRO:C	1:A:320:MET:N	2.73	0.41
1:A:184:THR:HB	1:A:185:LYS:H	1.69	0.40
1:A:203:HIS:HE1	1:A:205:ASN:HD22	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	263/280 (94%)	237 (90%)	21 (8%)	5 (2%)	6 29
1	B	261/280 (93%)	243 (93%)	15 (6%)	3 (1%)	12 40
All	All	524/560 (94%)	480 (92%)	36 (7%)	8 (2%)	8 33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	THR
1	A	157	ALA
1	A	185	LYS
1	B	185	LYS
1	B	184	THR
1	A	300	LEU
1	B	157	ALA
1	A	207	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	233/246 (95%)	204 (88%)	29 (12%)	4 16
1	B	230/246 (94%)	209 (91%)	21 (9%)	7 27
All	All	463/492 (94%)	413 (89%)	50 (11%)	5 20

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	135	MET
1	A	138	VAL
1	A	160	THR
1	A	173	VAL
1	A	179	GLN
1	A	181	ARG
1	A	182	LYS
1	A	183	LEU
1	A	184	THR
1	A	185	LYS
1	A	187	GLU
1	A	197	MET
1	A	202	GLN
1	A	208	ARG
1	A	218	LYS
1	A	221	LYS
1	A	234	THR
1	A	236	LYS
1	A	240	LYS
1	A	241	ARG
1	A	248	LYS
1	A	268	THR
1	A	277	LYS
1	A	283	ILE
1	A	301	MET
1	A	316	MET
1	A	362	THR
1	A	395	SER
1	B	138	VAL
1	B	151	ILE
1	B	165	LEU
1	B	173	VAL
1	B	175	TRP
1	B	176	CYS
1	B	179	GLN
1	B	181	ARG
1	B	182	LYS
1	B	183	LEU
1	B	185	LYS
1	B	187	GLU
1	B	255	ARG
1	B	268	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	277	LYS
1	B	301	MET
1	B	315	PHE
1	B	316	MET
1	B	353	ASN
1	B	359	ARG
1	B	392	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	205	ASN
1	B	205	ASN
1	B	401	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/280 (95%)	-0.79	0 100 100	34, 81, 135, 186	0
1	B	265/280 (94%)	-0.80	1 (0%) 89 83	48, 83, 141, 216	0
All	All	532/560 (95%)	-0.79	1 (0%) 92 88	34, 82, 138, 216	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	THR	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.